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Calculation of atomic energy levels for electronic configurations with one electron outside a nearly closed shell and two holes in this shell for LS and pair couplings

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SUMMARY

General formulae are given for the energy matrix of electronic configurations with two holes in a nearly closed shell and one electron outside the shell. The results are valid for arbitrary values of the angular momenta both of the electrons in the shell and of the electron outside the shell. If our formulae are specialized to the configurations $p^4 p$ and $p^4 d$ they agree with earlier results obtained by Yamanouchi [1] for the case of Russell-Saunders coupling. Our results also apply to the pair coupling scheme of Racah [2] and have been used to investigate the spectrum of singly ionized argon, ArII.

Introduction

The extended analysis of the spectrum of singly ionized argon, ArII, by Minnhagen has given a large number of new energy levels based on different $p^4 n l$ configurations. He was able to compare his experimental energy values with the theoretical ones given by Yamanouchi [1] for $p^4 p$ and $p^4 d$, but for the $p^4 f$ and $p^4 g$ configurations, for which he has found complete systems for several n values, no theory has previously been given.

In the present paper, a general treatment of $p^4 l$ configurations is undertaken. Our results agree with those of Yamanouchi for $l=1$ and $l=2$. For $l=3$ and $l=4$ the results are tabulated. The experimental data indicate that the configurations $p^4 l$ with $l=1$ and $l=2$ can be well approximated with the aid of Russell-Saunders coupling while the configurations with $l=3$ and $l=4$ are perhaps better described with the aid of the pair coupling scheme of Racah (i.e. $|(s_1\, s_2)\, S_{12},\ (l_1\, l_2)\, L_{12},\ J_{12},\ l_3,\ K,\ s_3,\ J\rangle$, cf. [2]). A detailed comparison between these results and experiments is published by Minnhagen in this issue of the Arkiv för Fysik. Our results are also valid for other systems containing two holes in a nearly closed shell and one outer electron.

To make our discussion reasonably self-contained we first compute the energy matrices for configurations consisting of 2 and 3 electrons outside closed shells.

Two electrons outside a closed shell

Let the electrons have angular momenta l_1 and l_2 (with components m_1 and m_2 in the z-direction). We combine their wave functions with the help of Clebsch-Gordan coefficients (our notation for these coefficients is similar to that of [3]) to a wave function with total angular momentum L.

$$|L\,M\rangle = \sum_{m_1 m_2} \langle l_1\, l_2\, m_1\, m_2 | L\, M\rangle \frac{1}{\sqrt{2}} [u_{l_1}^{m_1}(1)\, u_{l_2}^{m_2}(2)\, \chi_S^{ms}(12) - u_{l_1}^{m_1}(2)\, u_{l_2}^{m_2}(1)\, \chi_S^{ms}(21)] \tag{1}$$

where $\chi_S^{ms}(12)$ is the spin wave function of the particles 1 and 2.

We are interested in matrix elements of the type $\langle L\,M | \dfrac{e^2}{r_{12}} | L'\,M'\rangle$. These quantities are sums of expressions of the type $8^6 1$ in [3]. They are, as is well known, of two kinds, J and K (see [3] $8^6 12$), which are the Coulomb energy and the exchange energy respectively. Considering the first of these and using the formula on top of p. 175 in [3], we can write $8^6 1$ in [3] as

$$J = \delta_{SS'}\, \delta_{m_S m'_S} \sum_\lambda \sum_\mu F^\lambda \frac{4\pi}{2\lambda+1} (-1)^{m_1+m_2+\mu} \int d\Omega_1\, Y_{l_1}^{-m_1}(\Omega_1)\, Y_\lambda^{-\mu}(\Omega_1)\, Y_l^{m'_1}(\Omega_1) \cdot$$
$$\cdot \int d\Omega_2\, Y_{l_2}^{-m_2}(\Omega_2)\, Y_\lambda^{\mu}(\Omega_2)\, Y_{l_2}^{m'_2}(\Omega_2) \tag{2}$$

where Y_l^m denotes the conventional spherical harmonic with phase factor as defined in [4] and F^λ is given by $8^6 15\,a$ in [3]. We have

$$\int d\Omega\, Y_{l_1}^{m_1}(\Omega)\, Y_{l_2}^{m_2}(\Omega)\, Y_{l_3}^{m_3}(\Omega) = \left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right]^{\frac{1}{2}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \tag{3}$$

(See [4] p. 63 and (3.7) where the Wigner $3-j$ symbol $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ is defined.)

Consequently, we can write

$$J = \delta_{SS'}\, \delta_{m_S m'_S} \sum_\lambda \sum_\mu \alpha_\lambda F^\lambda \tag{4}$$

where

$$\alpha_\lambda = (2l_1+1)(2l_2+1) \begin{pmatrix} l_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_1 & \lambda \\ -m_1 & m'_1 & -\mu \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ -m_2 & m'_2 & \mu \end{pmatrix}. \tag{5}$$

Analogously, we get for the second type of term in $8^6 12$

$$K = \delta_{SS'}\, \delta_{m_S m'_S} \sum_\lambda \sum_\mu \beta_\lambda G^\lambda \tag{6}$$

where G^λ is defined in $8^6 15\,\mathrm{b}$ in [3] and

$$\beta_\lambda = (-1)^S (2l_1+1)(2l_2+1)\cdot$$
$$\cdot \begin{pmatrix} l_1 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \lambda \\ -m_1 & m_2' & -\mu \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \lambda \\ m_1' & -m_2 & \mu \end{pmatrix} (-1)^{m_1+m_2+\mu}. \quad (7)$$

Collecting (1), (4) and (6) we get

$$\langle L M \,|\, \frac{e^2}{r_{12}} \,|\, L' M' \rangle = \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \langle l_1\, l_2\, m_1\, m_2 \,|\, L M \rangle \langle l_1\, l_2\, m_1'\, m_2' \,|\, L M \rangle \cdot$$
$$\cdot \sum_\lambda \sum_\mu (\alpha_\lambda F^\lambda + \beta_\lambda G^\lambda)\, \delta_{LL'}\, \delta_{MM'}\, \delta_{SS'}\, \delta_{m_S m_S'} = \left(\sum_\lambda f_\lambda F^\lambda + (-1)^S \sum_\lambda g_\lambda G^\lambda\right) \delta_{LL'}\, \delta_{MM'}\, \delta_{SS'}\, \delta_{m_S m_S'}. \quad (8)$$

The relation between Wigner's $3-j$ symbols and the Clebsch-Gordan coefficients (see [4] p. 46) gives us

$$f_\lambda = \sum_{\substack{m_1 m_2 \\ m_1' m_2' \\ \mu}} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L \\ m_1' & m_2' & -M \end{pmatrix} (2L+1)(2l_1+1)(2l_2+1)\cdot$$
$$\cdot \begin{pmatrix} l_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_1 & \lambda \\ -m_1 & m_1' & -\mu \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ -m_2 & m_2' & \mu \end{pmatrix} (-1)^{m_1+m_2+\mu}. \quad (9)$$

Because of symmetry, f_λ must be independent of M and we can extend the summation to M if we divide by the number of terms in this sum, $2L+1$.

$$f_\lambda = (2l_1+1)\,(2l_2+1) \begin{pmatrix} l_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} (-1)^{l_1+l_2+L} \sum_{\substack{m_1 m_2 \\ m_1' m_2' \\ \mu\, M}} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix}\cdot$$
$$\cdot \begin{pmatrix} l_1 & l_2 & L \\ -m_1' & -m_2' & M \end{pmatrix} \begin{pmatrix} l_1 & l_1 & \lambda \\ -m_1 & m_1' & -\mu \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ -m_2 & m_2' & \mu \end{pmatrix} (-1)^{m_1+m_2+\mu}. \quad (10)$$

We have used the symmetry property (3.7.6) in [4] for the second $3-j$ symbol in the sum in order to get the sum in a form suitable for the next step of the calculation. Introducing Wigner's $6-j$ symbol $\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix}$ (see [4] Ch. 6) and using the formula (6.2.3) of [4], we see that

$$f_\lambda = (2l_1+1)(2l_2+1) \begin{pmatrix} l_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_1 & l_2 & L \\ l_2 & l_1 & \lambda \end{Bmatrix} (-1)^L. \quad (11)$$

Analogously, we get

$$g_\lambda = (2l_1+1)(2l_2+1) \left[\begin{pmatrix} l_1 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \right]^2 \begin{Bmatrix} l_1 & l_2 & L \\ l_1 & l_2 & \lambda \end{Bmatrix}. \quad (12)$$

The results we have found here and those we shall find in the next section have earlier been obtained by Racah, [5] and [6], but we give them in a slightly different form, which is useful for our later applications.

Three electrons outside a closed shell

In this case we calculate

$$\langle L\,M\,|\frac{e^2}{r_{12}}+\frac{e^2}{r_{23}}+\frac{e^2}{r_{13}}|\,L'\,M'\rangle =$$

$$=\langle L\,M\,|\,H_{12}\,|\,L'\,M'\rangle+\langle L\,M\,|\,H_{23}\,|\,L'\,M'\rangle+\langle L\,M\,|\,H_{13}\,|\,L'\,M'\rangle. \quad (13)$$

(We still consider Russell-Saunders coupling.)

Here, we shall couple the angular momenta l_1, l_2 and l_3 to a resultant L. This can be done in different ways (see [4] Ch. 6). The relation between states obtained by coupling three angular momenta in different orders to give the same total angular momentum is illustrated by the relation (6.1.5) in [4] which can be written

$$|\,(j_1\,j_2)\,j_{12},\,j_3,\,J\rangle=\sum_{j_{23}}(-1)^{j_1+j_2+j_3+J}\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23}\end{Bmatrix}[(2\,j_{12}+1)\,(2\,j_{23}+1)]^{\frac{1}{2}}\,|\,j_1,\,(j_2\,j_3)\,j_{23},\,J\rangle \quad (14)$$

and which is frequently used in the following.

We start with

$$\langle L\,M\,|\,H_{12}\,|\,L'\,M'\rangle=\langle (l_1\,l_2)\,L_{12},\,l_3,\,L\,|\frac{e^2}{r_{12}}|\,(l_1\,l_2)\,L'_{12},\,l_3,\,L'\rangle =$$

$$=\langle (l_1\,l_2)\,L_{12}\,|\frac{e^2}{r_{12}}|\,(l_1\,l_2)\,L'_{12}\rangle\,\delta_{LL'}\,\delta_{MM'}=$$

$$=\delta_{LL'}\,\delta_{MM'}\,\delta_{L_{12}L'_{12}}\,\delta_{M_{12}M'_{12}}\,\delta_{S_{12}S'_{12}}\,\delta_{m_{S_{12}}m'_{S_{12}}}\sum_{\lambda}(f_\lambda\,F^\lambda+(-1)^{S_{12}}\,g_\lambda\,G^\lambda) \quad (15)$$

where f_λ and g_λ are given in Eqs. (11) and (12) above.

The second term in (13) is given by

$$\langle L\,M\,|H_{23}\,|\,L'\,M'\rangle=\langle (l_1\,l_2)\,L_{12},\,l_3,\,L\,|\frac{e^2}{r_{23}}|\,(l_1\,l_2)L'_{12},\,l_3,\,L'\rangle \quad (16)$$

or, if we write out explicitly the spin quantum numbers of the states

$$\langle L\,M\,|\,H_{23}\,|\,L'\,M'\rangle =$$

$$=\langle (l_1\,l_2)\,L_{12},\,l_3,\,L,\,((s_1\,s_2)\,S_{12},\,s_3)\,S,\,J\,|\frac{e^2}{r_{23}}|\,(l_1\,l_2)\,L'_{12},\,l_3,\,L',\,((s_1,\,s_2)\,S'_{12},\,s_3)\,S',\,J\rangle =$$

$$=\delta_{LL'}\,\delta_{MM'}\sum_{\substack{L_{23}L'_{23}\\ S_{23}S'_{23}}}\begin{Bmatrix} l_1 & l_2 & L_{12} \\ l_3 & L & L_{23}\end{Bmatrix}\begin{Bmatrix} l_1 & l_2 & L'_{12} \\ l_3 & L & L'_{23}\end{Bmatrix}[(2\,L_{12}+1)\,(2\,L'_{12}+1)\,(2\,L_{23}+1)\,(2\,L'_{23}+1)]^{\frac{1}{2}}\,\cdot$$

$$\cdot \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S_{12} \\ \frac{1}{2} & S & S_{23} \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S'_{12} \\ \frac{1}{2} & S & S'_{23} \end{Bmatrix} [(2\,S_{12}+1)\,(2\,S'_{12}+1)\,(2\,S_{23}+1)\,(2\,S'_{23}+1)]^{\frac{1}{2}} \cdot$$

$$\cdot\, \delta_{L_{23}L'_{23}} \sum_{\lambda} \{f_\lambda\,(l_2\,l_3\,L_{23})\,F^\lambda\,(23) + g_\lambda\,(l_2\,l_3\,L_{23})\,G^\lambda\,(23)\,(-1)^{S_{23}}\}\,\delta_{S_{23}S'_{23}} =$$

$$= \delta_{LL'}\,\delta_{MM'} \sum_{\lambda} (\bar{f}_\lambda\,F^\lambda + \bar{g}_\lambda\,G^\lambda) \qquad (17)$$

where we have used (14).

$$\bar{f}_\lambda = \delta_{S_{12}S'_{12}}\,[(2\,L_{12}+1)\,(2\,L'_{12}+1)]^{\frac{1}{2}}\,(2\,l_2+1)\,(2\,l_3+1) \begin{pmatrix} l_2 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_3 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \cdot$$

$$\cdot \sum_{L_{23}} (-1)^{L_{23}}\,(2\,L_{23}+1) \begin{Bmatrix} l_1 & l_2 & L_{12} \\ l_3 & L & L_{23} \end{Bmatrix} \begin{Bmatrix} l_1 & l_2 & L'_{12} \\ l_3 & L & L_{23} \end{Bmatrix} \begin{Bmatrix} l_2 & L_{23} & l_3 \\ l_3 & \lambda & l_2 \end{Bmatrix}. \qquad (18\text{ a})$$

In the last $6-j$ symbol above we have used the symmetry property which allows us to interchange columns (see (6.2.4) in [4]).

$$\bar{f}_\lambda = [(2\,L_{12}+1)\,(2\,L'_{12}+1)]^{\frac{1}{2}}\,(2\,l_2+1)\,(2\,l_3+1) \begin{pmatrix} l_2 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_3 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} L_{12} & \lambda & L'_{12} \\ l_3 & L & l_3 \end{Bmatrix} \cdot$$

$$\cdot \begin{Bmatrix} L_{12} & \lambda & L'_{12} \\ l_2 & l_1 & l_2 \end{Bmatrix} (-1)^{L_{12}+L'_{12}+l_1+L}\,\delta_{S_{12}S'_{12}}. \qquad (18\text{ b})$$

To obtain Eq. (18 a) we have used the formula

$$\sum_{S_{23}} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S_{12} \\ \frac{1}{2} & S & S_{23} \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S'_{12} \\ \frac{1}{2} & S & S_{23} \end{Bmatrix} (2\,S_{23}+1)\,(2\,S_{12}+1) = \delta_{S_{12}S'_{12}}. \qquad (19)$$

((6.2.9) in [4]) to evaluate the sum over the spin states. Furthermore, Eq. (6.2.12) in [4] has been used to perform the summation over L_{23}. In a similar way we find with the aid of (6.2.11) in [4] the following expression for $\bar{g}_\lambda$.

$$\bar{g}_\lambda = (-1)^{S_{12}+S'_{12}} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S_{12} \\ \frac{1}{2} & S & S'_{12} \end{Bmatrix} [(2\,S_{12}+1)\,(2\,S'_{12}+1)]^{\frac{1}{2}}\,(2\,l_2+1)\,(2\,l_3+1) \cdot$$

$$\cdot [(2L_{12}+1)\,(2\,L'_{12}+1)]^{\frac{1}{2}} \left[\begin{pmatrix} l_2 & l_3 & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 \sum_{L_{23}} (2\,L_{23}+1) \begin{Bmatrix} l_1 & l_2 & L_{12} \\ l_3 & L & L_{23} \end{Bmatrix} \begin{Bmatrix} l_1 & l_2 & L'_{12} \\ l_3 & L & L_{23} \end{Bmatrix} \begin{Bmatrix} l_2 & l_3 & L_{23} \\ l_2 & l_3 & \lambda \end{Bmatrix}. \qquad (20)$$

This formula can also be expressed with the help of Wigner's $9-j$ symbol (see [4], 6.4.):

$$\bar{g}_\lambda = (-1)^{S_{12}+S'_{12}} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S_{12} \\ \frac{1}{2} & S & S'_{12} \end{Bmatrix} [(2\,S_{12}+1)\,(2\,S'_{12}+1)]^{\frac{1}{2}}\,(2\,l_2+1)\,(2\,l_3+1) \cdot$$

$$\cdot [(2\,L_{12}+1)\,(2\,L'_{12}+1)]^{\frac{1}{2}} \left[\begin{pmatrix} l_2 & l_3 & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 \begin{Bmatrix} l_2 & l_3 & \lambda \\ l_1 & L'_{12} & l_2 \\ L_{12} & L & l_3 \end{Bmatrix}. \qquad (20\text{ a})$$

However, since the $9-j$ symbols are not very extensively tabulated, (20) is the formula to be used for numerical evaluation of $\bar{g}_\lambda$.

For reasons of symmetry, the matrix elements of H_{13} are the same as the matrix elements of H_{23}. The total energy is hence given by the sum of Eq. (15) and twice the expression in Eq. (17).

Almost closed electron shell

Now, we shall make calculations, similar to the preceding ones, for holes in electron shells instead of particles outside closed shells. For one hole and one electron outside a closed shell, calculations have been done previously by Condon and Shortley [3], Shortley and Fried [7] and Racah [6] for some special cases. Racah also treats the $d^8 p$ configuration in [6]. We shall do the corresponding calculations in a more general way, which will be easily modified to fit our case of 2 holes and 1 outer electron, first for LS coupling and later on for pair coupling.

A closed shell with a given l consists of $2(2l+1)=n$ electrons. Let u_i $(i=1, \ldots, n)$ be their wave functions. If $\chi(+)$ denotes spin up and $\chi(-)$ spin down, we introduce the notation

$$u_{2j+1} = \varphi(r)\, Y_l^{l-j}\, \chi(+), \tag{21}$$

$$u_{2(j+1)} = \varphi(r)\, Y_l^{l-j}\, \chi(-). \tag{22}$$

Applying the spin operators S_+ and S_- and the angular momentum operators L_+ and L_- $(S_\pm = S_x \pm i S_y,\ L_\pm = L_x \pm i L_y)$ we have

$$S_+ u_i = \begin{cases} u_{i-1} & \text{if } i \text{ is even,} \qquad (23\text{ a}) \\ 0 & \text{if } i \text{ is odd.} \qquad (23\text{ b}) \end{cases}$$

$$S_- u_i = \begin{cases} 0 & \text{if } i \text{ is even,} \qquad (24\text{ a}) \\ u_{i+1} & \text{if } i \text{ is odd.} \qquad (24\text{ b}) \end{cases}$$

$$L_+ u_i = \sqrt{(l-m_i)(l+m_i+1)}\, u_{i-2} \tag{25}$$

and

$$L_- u_i = \sqrt{(l+m_i)(l-m_i+1)}\, u_{i+2}. \tag{26}$$

where $m_i = l-j$ both for $i=2j+1$ and for $i=2(j+1)$.

We define (with P = the permutation operator of [3] p. 162).

$$|\phi\rangle = \frac{1}{\sqrt{n!}} \sum_P (-1)^P P(u_1(1)\, u_2(2) \ldots u_n(n)) \tag{27}$$

(the wave function of a closed shell), and

$$|\phi_i\rangle = \frac{1}{\sqrt{(n-1)!}} \sum_P (-1)^P P(u_1(1) \ldots u_{i-1}(i-1)\, u_{i+1}(i) \ldots u_n(n-1)) \tag{28}$$

(the wave function of a shell with one particle missing).

Applying spin and angular momentum operators to $|\phi_i\rangle$ we get

$$L_z|\phi_i\rangle = -m_i|\phi_i\rangle. \tag{29}$$

$$S_z|\phi_i\rangle = (-1)^i \tfrac{1}{2}|\phi_i\rangle. \tag{30}$$

$$S_+|\phi_i\rangle = \begin{cases} 0 \text{ if } i \text{ is even} & (31\text{ a}) \\ |\phi_{i+1}\rangle \text{ if } i \text{ is odd.} & (31\text{ b}) \end{cases}$$

$$S_-|\phi_i\rangle = \begin{cases} |\phi_{i-1}\rangle \text{ if } i \text{ is even,} & (32\text{ a}) \\ \quad 0 \quad \text{if } i \text{ is odd.} & (32\text{ b}) \end{cases}$$

$$L_+|\phi_i\rangle = \sqrt{(l-m_{i+2})(l+m_{i+2}+1)}\frac{1}{\sqrt{(n-1)!}}\sum_P(-1)^P P(u_1(1)\dots u_{i-1}(i-1)\cdot$$

$$\cdot u_i(i+1)\,u_{i+1}(i)\,u_{i+3}(i+2)\dots u_n(n-1)) = \sqrt{(l-m_{i+2})(l+m_{i+2}+1)}\frac{1}{\sqrt{(n-1)!}}\cdot$$

$$\cdot\sum_P(-1)^{P+1}P(u_1(1)\dots u_{i-1}(i-1)\,u_i(i)\,u_{i+1}(i+1)\,u_{i+3}(i+2)\dots u_n(n-1)) =$$

$$= -\sqrt{(l-m_{i+2})(l+m_{i+2}+1)}\,|\phi_{i+2}\rangle. \tag{33}$$

Because $m_{i+2} = m_i - 1$ the square root in front of $|\phi_{i+2}\rangle$ can be written

$$\sqrt{(l+(-m_i)+1)(l-(-m_i))}\,.$$

Consequently

$$|\phi_i\rangle = (-1)^{m_i}|l,\ -m_i,\ \tfrac{1}{2},\ (-1)^i\tfrac{1}{2}\rangle \tag{34}$$

where, in particular, we note the phase factor $(-1)^{m_i}$.

Now we are going to calculate the energy matrix of a hole, i.e.

$$X_{ij} = \langle\phi_i|\sum_{k>l}\frac{e^2}{r_{kl}}|\phi_j\rangle. \tag{35}$$

As is well-known, this matrix is diagonal. We can verify this with the aid of the following explicit calculation. For $i \neq j$ we get

$$X_{ij} = \langle u_1(1)\dots u_{i-1}(i-1)\,u_{i+1}(i)\dots u_n(n-1)|\sum_{k>l}\frac{e^2}{r_{kl}}|\sum_P(-1)^P P(u_1(1)\dots u_{j-1}(j-1)\cdot$$

$$\cdot u_{j+1}(j)\dots u_n(n-1))\rangle = (-1)^{i+j}\sum_{k=1}^{n}\langle u_j(1)\,u_k(2)|\frac{e^2}{r_{12}}|u_i(1)\,u_k(2) - u_i(2)\,u_k(1)\rangle =$$

$$= (-1)^{i+j}\sum_{k=1}^{n}\sum_{\lambda}[a_\lambda F^\lambda\,\delta_{m_{s_i}m_{s_j}} - b_\lambda G^\lambda\,\delta_{m_{s_i}m_{s_k}}\,\delta_{m_{s_j}m_{s_k}}] \tag{36}$$

where

$$a_\lambda = (2l+1)^2\left[\begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0\end{pmatrix}\right]^2\begin{pmatrix} & & \lambda \\ -m_j & m_i & -\mu\end{pmatrix}\begin{pmatrix} l & l & \lambda \\ -m_k & m_k & \mu\end{pmatrix}(-1)^{m_j+m_k+\mu} \tag{37}$$

and $$b_\lambda = (2l+1)^2 \left[\begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 \begin{pmatrix} l & l & \lambda \\ -m_j & m_k & -\mu \end{pmatrix} \begin{pmatrix} l & l & \lambda \\ -m_k & m_i & \mu \end{pmatrix} (-1)^{m_k+m_j+\mu} \tag{38}$$

are obtained from Eqs. (5) and (7) above. Note, that the $3-j$ symbols in a_λ and b_λ vanish if $m_i \neq m_j$. Consequently $X_{ij}=0$ if $i \neq j$. If we calculate X_{ii} we get an expression dependent on l but not on i. This means that all holes in a shell have the same energy, that is

$$X_{ij} = \delta_{ij}\, 2l(2l+1) \left\{ 2F^0 - \sum_\lambda G^\lambda \left[\begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 \right\}. \tag{39}$$

We now turn to the case of one hole in the shell and one electron outside the shell. If we denote the latter electron with v, its angular momentum with l_v, and if the electron shell with one missing particle has the wave function $|\phi_i\rangle$, we get the total wave function

$$|\psi_i\rangle = \frac{1}{\sqrt{n\,!}} \sum_P (-1)^P P(u_1(1) \dots u_{i-1}(i-1)\, u_{i+1}(i) \dots u_n(n-1)\, v(n)) =$$

$$= \frac{(-1)^i}{\sqrt{n\,!}} \sum_P (-1)^P P(u_1(1) \dots u_{i-1}(i-1)\, v(i)\, u_{i+1}(i+1) \dots u_n(n)). \tag{40 a}$$

$$|\psi_j'\rangle = \frac{(-1)^j}{\sqrt{n\,!}} \sum_P (-1)^P P(u_1(1) \dots u_{j-1}(j-1)\, v'(j)\, u_{j+1}(j+1) \dots u_n(n)). \tag{40 b}$$

$$\begin{aligned}
\langle\psi_i| \sum_{k>l} \frac{e^2}{r_{kl}} |\psi_j'\rangle = {} & (-1)^{i+j+1} \langle v(1)\, u_j(2) | \frac{e^2}{r_{12}} | v'(1)\, u_i(2) - v'(2)\, u_i(1)\rangle + \\
& + \delta_{ij} \sum_{k=1}^{n} \langle v(1)\, u_k(2) | \frac{e^2}{r_{12}} | v'(1)\, u_k(2) - v'(2)\, u_k(1)\rangle + \\
& + \delta_{ij}\, \delta_{vv'} \sum_{k>l \neq i} \langle u_k(1)\, u_l(2) | \frac{e^2}{r_{12}} | u_k(1)\, u_l(2) - u_k(2)\, u_l(1)\rangle.
\end{aligned} \tag{41}$$

The second term in (41) can be rewritten as

$$\begin{aligned}
& \sum_{k=1}^{n} \langle v(1)\, u_k(2) | \frac{e^2}{r_{12}} | v'(1)\, u_k(2) - v'(2)\, u_k(1)\rangle = \\
& = \delta_{vv'} \left\{ 2(2l+1) F^0(l\, l_v) - (2l+1) \sum_\lambda \left[\begin{pmatrix} l_v & l & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 G^\lambda(l\, l_v) \right\}.
\end{aligned} \tag{42}$$

The third term in (41) is equal to $\delta_{ij}\, \delta_{vv'}\, X_{ii}$.
Inserting this in (41) we get

$$\langle\psi_i|\sum_{k>l}\frac{e^2}{r_{kl}}|\psi_j'\rangle=(-1)^{i+j+1}\langle v(1)\,u_j(2)|\frac{e^2}{r_{12}}|v'(1)\,u_i(2)-v'(2)\,u_i(1)\rangle+$$

$$+\delta_{ij}\,\delta_{vv'}(2l+1)\left\{4l\,F^0(l\,l)+2F^0(l\,l_v)-2l\sum_\lambda G^\lambda(l\,l)\left[\begin{pmatrix}l & l & \lambda\\ 0 & 0 & 0\end{pmatrix}\right]^2-\right.$$

$$\left.-\sum_\lambda G^\lambda(l\,l_v)\left[\begin{pmatrix}l_v & l & \lambda\\ 0 & 0 & 0\end{pmatrix}\right]^2\right\}. \tag{43}$$

We see that $\langle\psi_i|\sum_{k>l}\frac{e^2}{r_{kl}}|\psi_j'\rangle$ consists of two terms, one of which is dependent on l and l_v but not on i or j, and which is a kind of zero-point energy. This expression does not interest us here and we disregard it from now on. Consequently, we write

$$\langle\psi_i|\sum_{k>l}\frac{e^2}{r_{kl}}|\psi_j'\rangle\sim(-1)^{i+j+1}\langle v(1)\,u_j(2)|\frac{e^2}{r_{12}}|v'(1)\,u_i(2)-v'(2)\,u_i(1)\rangle. \tag{44}$$

With the aid of the same technique as before, we get

$$\langle\psi_i|\sum_{k>l}\frac{e^2}{r_{kl}}|\psi_j'\rangle=(-1)^{m_{s_i}-m_{s_j}+1}\left\{\delta_{m_{s_v}m_{s_{v'}}}\,\delta_{m_{s_i}m_{s_j}}\sum_\lambda a_\lambda F^\lambda-\delta_{m_{s_v}m_{s_i}}\,\delta_{m_{s_{v'}}m_{s_j}}\sum_\lambda b_\lambda G^\lambda\right\} \tag{45}$$

where

$$a_\lambda=(2l+1)(2l_v+1)\begin{pmatrix}l & l & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_v & l_v & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l & l & \lambda\\ -m_j & m_i & -\mu\end{pmatrix}\begin{pmatrix}l_v & l_v & \lambda\\ -m_v & m_{v'} & \mu\end{pmatrix}(-1)^{m_j+m_v+\mu}, \tag{46}$$

$$b_\lambda=(2l+1)(2l_v+1)\left[\begin{pmatrix}l & l_v & \lambda\\ 0 & 0 & 0\end{pmatrix}\right]^2\begin{pmatrix}l & l_v & \lambda\\ -m_j & m_{v'} & -\mu\end{pmatrix}\begin{pmatrix}l_v & l & \lambda\\ -m_v & m_i & \mu\end{pmatrix}(-1)^{m_j+m_v+\mu}. \tag{47}$$

The states $|\psi_i\rangle$ in Eq. (40) can be added with Clebsch-Gordan coefficients to give states with definite total angular momentum. Noting the factor $(-1)^{m_i}$ in Eq. (34) we get

$$|LM,S\,M_S\rangle=\sum_{\substack{m_im_v\\ m_{s_i}m_{s_v}}}\langle l\,l_v-m_i\,m_v|LM\rangle\langle\tfrac12\,\tfrac12-m_{s_i}\,m_{s_v}|S\,M_S\rangle(-1)^{m_i}|\psi_i\rangle. \tag{48}$$

With the aid of the two formulae

$$\sum_{\substack{m_{s_i}m_{s_v}\\ m_{s_j}m_{s_{v'}}}}\langle\tfrac12\,\tfrac12-m_{s_i}\,m_{s_v}|S\,M_S\rangle\langle\tfrac12\,\tfrac12-m_{s_j}\,m_{s_{v'}}|S'\,M_S'\rangle\cdot\begin{cases}\delta_{m_{s_i}m_{s_j}}\,\delta_{m_{s_v}m_{s_{v'}}}\\ \delta_{m_{s_i}m_{s_v}}\,\delta_{m_{s_j}m_{s_{v'}}}\end{cases}=$$

$$=\begin{cases}-\delta_{SS'}\,\delta_{M_SM_S'} & \text{(49 a)}\\ -2\,\delta_{SS'}\,\delta_{M_SM_S'}\,\delta_{S0}\,\delta_{M_S0} & \text{(49 b)}\end{cases}$$

Tables 1. Coefficients for the electrostatic integrals F^λ and G^λ in Russell-Saunders coupling when there are two holes in a p-shell and one electron outside the shell. The total angular momentum is $\mathcal{L}$. The parents of the terms are used for classification of the levels.

1 a. Diagonal terms (doublets).

Parents	$\mathcal{L}$	$\bar{f}_0$	$\bar{f}_2$	$\bar{g}_{l-1}$	$\bar{g}_{l+1}$
^1S	l	1	0	$\frac{l}{2(4l^2-1)}$	$\frac{l+1}{2(2l+1)(2l+3)}$
^3P	$l+1$	1	$-\frac{l}{10(2l+3)}$	0	$\frac{9(l+2)}{4(2l+3)^2}$
	l	1	$\frac{1}{10}$	$\frac{9(l+1)}{4(4l^2-1)}$	$\frac{9l}{4(2l+1)(2l+3)}$
	$l-1$	1	$-\frac{l+1}{10(2l-1)}$	$\frac{9(l-1)}{4(2l-1)^2}$	0
^1D	$l+2$	1	$\frac{l}{5(2l+3)}$	0	$\frac{3(l+1)}{2(2l+3)^2}$
	$l+1$	1	$-\frac{l+6}{10(2l+3)}$	0	$\frac{3l}{4(2l+3)^2}$
	l	1	$-\frac{4l^2+4l-15}{10(2l-1)(2l+3)}$	$\frac{(l+1)(2l+3)}{4(2l-1)(4l^2-1)}$	$\frac{l(2l-1)}{4(2l+1)(2l+3)^2}$
	$l-1$	1	$-\frac{l-5}{10(2l-1)}$	$\frac{3(l+1)}{4(2l-1)^2}$	0
	$l-2$	1	$\frac{l+1}{5(2l-1)}$	$\frac{3l}{2(2l-1)^2}$	0

For the quartets, $\bar{f}_0$ and $\bar{f}_2$ are the same as for the doublets but $\bar{g}_{l-1} = \bar{g}_{l+1} = 0$.

we finally get

$$\langle L\,M, S\,M_S | \sum_{k>l} \frac{e^2}{r_{kl}} | L'\,M', S'\,M'_S \rangle = \delta_{SS'}\,\delta_{M_S M'_S}\,\delta_{LL'}\,\delta_{MM'} \cdot$$

$$\cdot \{ -\sum f_\lambda F^\lambda + \delta_{S0} \sum g_\lambda G^\lambda \} \qquad (50)$$

with

$$f_\lambda = \sum_{\substack{m_i m_v \\ m_j m_{v'}}} \langle l\,l_v - m_i\,m_v | L\,M \rangle \langle l\,l_v - m_j\,m_{v'} | L\,M \rangle\, a_\lambda =$$

$$= (2l+1)(2l_v+1) \begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_v & l_v & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l & L & l_v \\ l_v & \lambda & l \end{Bmatrix} (-1)^L \qquad (51)$$

which is the same as f_λ earlier in Eq. (11).

1 b. Non-diagonal terms (doublets).

Parents		$\mathcal{L}$	$\bar{f}_2$	$\bar{g}_{l-1}$	$\bar{g}_{l+1}$
^3P	^1D	$l+1$	0	0	$-\frac{3\sqrt{3}\sqrt{l(l+2)}}{4(2l+3)^2}$
^1S	^3P	l	0	$\frac{3\sqrt{l(l+1)}}{2\sqrt{2}(4l^2-1)}$	$-\frac{3\sqrt{l(l+1)}}{2\sqrt{2}(2l+1)(2l+3)}$
^1S	^1D	l	$\frac{\sqrt{2}\sqrt{l(l+1)}}{5\sqrt{(2l+3)(2l-1)}}$	$\frac{\sqrt{l(2l+3)(l+1)}}{2\sqrt{2}(2l-1)^{3/2}(2l+1)}$	$\frac{\sqrt{l(2l-1)(l+1)}}{2\sqrt{2}(2l+1)(2l+3)^{3/2}}$
^3P	^1D	l	0	$\frac{3(l+1)\sqrt{2l+3}}{4(2l+1)(2l-1)^{3/2}}$	$-\frac{3l\sqrt{2l-1}}{4(2l+1)(2l+3)^{3/2}}$
^3P	^1D	$l-1$	0	$\frac{3\sqrt{3}\sqrt{l^2-1}}{4(2l-1)^2}$	0

$$g_\lambda = 2(2l+1)(2l_v+1)\left[\begin{pmatrix} l & l_v & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 \sum_{\substack{m_i m_v \\ m_j m_{v'}}} \langle l\, l_v - m_i\, m_v | L\, M\rangle \langle l\, l_v - m_j\, m_{v'} | L\, M\rangle \cdot$$

$$\cdot \begin{pmatrix} l & l_v & \lambda \\ -m_j & m_{v'} & -\mu \end{pmatrix} \begin{pmatrix} l_v & l & \lambda \\ -m_v & m_i & \mu \end{pmatrix} (-1)^{m_i+m_v+\mu}. \tag{52}$$

Which can be simplified to

$$g_\lambda = \frac{2}{2L+1}(2l+1)(2l_v+1)\left[\begin{pmatrix} l & l_v & L \\ 0 & 0 & 0 \end{pmatrix}\right]^2 \delta_{L\lambda} \tag{53}$$

with the aid of Eqs. (3.7.3) and (3.7.8) in [4]. Because in our case of ArII there are 2 holes in the shell and one electron outside it, we must go one step further as in the earlier case of three electrons and calculate the corresponding $\bar{f}_\lambda$ and $\bar{g}_\lambda$ here. The angular momentum, to which the holes and the outer electron are combined here, is $\mathcal{L}$ and the resulting spin is S. Using again formula (14) we get

$$\bar{f}_\lambda = [(2L_{12}+1)(2L'_{12}+1)]^{\frac{1}{2}}(2l+1)(2l_v+1)\begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_v & l_v & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} L_{12} & \lambda & L'_{12} \\ l_v & \mathcal{L} & l_v \end{Bmatrix} \cdot$$

$$\cdot \begin{Bmatrix} L_{12} & \lambda & L'_{12} \\ l & l & l \end{Bmatrix} (-1)^{L_{12}+L'_{12}+l+\mathcal{L}} \delta_{S_{12}S'_{12}} \tag{54}$$

and $$\bar{g}_\lambda = \tfrac{1}{2}[(2L_{12}+1)(2L'_{12}+1)(2S_{12}+1)(2S'_{12}+1)]^{\frac{1}{2}}(2l+1)(2l_v+1) \cdot$$

$$\cdot \begin{Bmatrix} l & l & L_{12} \\ l_v & \mathcal{L} & \lambda \end{Bmatrix}\begin{Bmatrix} l & l & L'_{12} \\ l_v & \mathcal{L} & \lambda \end{Bmatrix}\left[\begin{pmatrix} l & l_v & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 (-1)^{S_{12}+S'_{12}} \delta_{S\frac{1}{2}}. \tag{55}$$

The total energy is given by $2\sum_\lambda(-\bar{f}_\lambda F^\lambda + \bar{g}_\lambda G^\lambda)$ + energy of parent ion.

Tables 2 a, b, c, d. Coefficients for the electrostatic integrals F^λ and G^λ in pair coupling (i.e. $|(s_1 s_2) S_{12}, (l_1 l_2) L_{12}, J_{12}, l_3, K, s_3, J\rangle$ cf. [2]) when there are two holes in a p-shell and one electron outside the shell.

2 a. Diagonal $\bar{f}'_\lambda$.

Parents	J_{12}	K	$2\bar{f}'_2$	$l=3$	$l=4$
^1S	0	l	0	0	0
^3P	0	l	0	0	0
	1	$l+1$	$\frac{l}{10(2l+3)}$	$\frac{1}{30}$	$\frac{2}{55}$
		l	$-\frac{1}{10}$	$-\frac{1}{10}$	$-\frac{1}{10}$
		$l-1$	$\frac{l+1}{10(2l-1)}$	$\frac{2}{25}$	$\frac{1}{14}$
	2	$l+2$	$-\frac{l}{5(2l+3)}$	$-\frac{1}{15}$	$-\frac{4}{55}$
		$l+1$	$\frac{l+6}{10(2l+3)}$	$\frac{1}{10}$	$\frac{1}{11}$
		l	$-\frac{15-4l(l+1)}{10(2l-1)(2l+3)}$	$\frac{11}{150}$	$\frac{13}{154}$
		$l-1$	$\frac{l-5}{10(2l-1)}$	$-\frac{1}{25}$	$-\frac{1}{70}$
		$l-2$	$-\frac{l+1}{5(2l-1)}$	$-\frac{4}{25}$	$-\frac{1}{7}$
^1D	2	$l+2$	$\frac{2l}{5(2l+3)}$	$\frac{2}{15}$	$\frac{8}{55}$
		$l+1$	$-\frac{l+6}{5(2l+3)}$	$-\frac{1}{5}$	$-\frac{2}{11}$
		l	$-\frac{4l(l+1)-15}{5(2l-1)(2l+3)}$	$-\frac{11}{75}$	$-\frac{13}{77}$
		$l-1$	$-\frac{l-5}{5(2l-1)}$	$\frac{2}{25}$	$\frac{1}{35}$
		$l-2$	$\frac{2(l+1)}{5(2l-1)}$	$\frac{8}{25}$	$\frac{2}{7}$

$\bar{f}'_2$ is the same for $J=K+\frac{1}{2}$ and for $J=K-\frac{1}{2}$. All $\bar{f}'_0=1$.

2 b. Non-diagonal $\bar{f}'_\lambda$.

Parents		K	J_{12}	J'_{12}	$2\bar{f}'_2$	$l=3$	$l=4$
^1S	^1D	l	0	2	$\frac{2\sqrt{2}\sqrt{l(l+1)}}{5\sqrt{(2l-1)(2l+3)}}$	$\frac{4\sqrt{30}}{75}$	$\frac{4\sqrt{770}}{385}$
^3P	^3P	l	0	2	$-\frac{\sqrt{2}\sqrt{l(l+1)}}{5\sqrt{(2l-1)(2l+3)}}$	$-\frac{2\sqrt{30}}{75}$	$-\frac{2\sqrt{770}}{385}$
		$l+1$	1	2	$-\frac{3\sqrt{l(l+2)}}{10(2l+3)}$	$-\frac{\sqrt{15}}{30}$	$-\frac{3\sqrt{6}}{55}$
		l	1	2	$\frac{3\sqrt{3}}{10\sqrt{(2l-1)(2l+3)}}$	$\frac{\sqrt{15}}{50}$	$\frac{3\sqrt{231}}{770}$
		$l-1$	1	2	$\frac{3\sqrt{(l-1)(l+1)}}{10(2l-1)}$	$\frac{3\sqrt{2}}{25}$	$\frac{3\sqrt{15}}{70}$

All $\bar{f}'_0=0$.

The two formulae above are very convenient for a numerical evaluation of the constants $\bar{f}_\lambda$ and $\bar{g}_\lambda$ when a table of the Wigner $3-j$ and $6-j$ symbols is available. For the particular case of ionized argon (ArII) we have $l=1$ and an arbitrary value of l_v. For this case, the tables given at the end of ref. [4] are sufficient for an evaluation of $\bar{f}_\lambda$ and $\bar{g}_\lambda$.[1] The result is given in table 1. The states are classified with the aid of the quantum numbers of the "parent ion", i.e. with the aid of S_{12} and L_{12} together with the total orbital momentum $\mathfrak{L}$. The index λ takes on only two different values. For the ^1S state of the parent ion we have only one state (a doublet) with $\mathfrak{L}=1$ for ArII. For the ^3P state of the parent, we have (in general) three possible values of $\mathfrak{L}$, viz. $\mathfrak{L}=l$ and $\mathfrak{L}=l\pm1$. Furthermore, these states can be either doublets or quartets. Finally, the parent state ^1D gives rise, in general, to 5 values of $\mathfrak{L}$, viz. $\mathfrak{L}=l$, $\mathfrak{L}=l\pm1$ and $\mathfrak{L}=l\pm2$. They are all doublets. In the special case that $l=1$, the quantum number $\mathfrak{L}$ can only have the values 3, 2 or 1.

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[1] In the tables of $6-j$ symbols of [4] we have found a couple of misprints which should be pointed out. First, on p. 131 in $\begin{Bmatrix} a & b & c \\ 2 & c-2 & b \end{Bmatrix}$ a factor $(s-2b-1)^{\frac{1}{2}}$ in the numerator has been omitted. Second, $\begin{Bmatrix} a & b & c \\ 2 & c-1 & b \end{Bmatrix}$ on. p. 132 should be

$$(-1)^s\, 2\cdot\frac{[(a+b+1)(a-b)-c^2+1]\,[6(s+1)(s-2a)(s-2b)(s-2c+1)]^{\frac{1}{2}}}{[(2b-1)\,2b\,(2b+1)(2b+2)(2b+3)(2c-2)(2c-1)\,2c\,(2c+1)(2c+2)]^{\frac{1}{2}}}.$$

The latter $6-j$ symbol is given correctly in Edmond's earlier version of [4], i.e. his lecture notes "Angular momentum in quantum mechanics", CERN-Publications 55-26.

2c. Diagonal $\bar{g}'_{\lambda}$.

Parents	J_{12}	K	J	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$
^1S	0	l	$K\pm\frac{1}{2}$	$\frac{2l}{4l^2-1}$	$\frac{6}{35}$	$\frac{8}{63}$	$\frac{2(l+1)}{(2l+1)(2l+3)}$	$\frac{8}{63}$
^3P	0	l	$K+\frac{1}{2}$	$\frac{l}{4l^2-1}$	$\frac{3}{35}$	$\frac{4}{63}$	$\frac{3l+2}{(2l+1)(2l+3)}$	$\frac{11}{63}$
		l	$K-\frac{1}{2}$	$\frac{3l+1}{4l^2-1}$	$\frac{2}{7}$	$\frac{13}{63}$	$\frac{l+1}{(2l+1)(2l+3)}$	$\frac{4}{63}$
	1	$l+1$	$K+\frac{1}{2}$	0	0	0	$\frac{3(l+2)}{2(2l+3)^2}$	$\frac{5}{54}$
		$l+1$	$K-\frac{1}{2}$	$\frac{3l(2l+3)}{2(l+1)(4l^2-1)}$	$\frac{81}{280}$	$\frac{22}{105}$	$\frac{3(6l^3+19l^2+20l+8)}{2(l+1)(2l+1)(2l+3)^2}$	$\frac{401}{1512}$
		l	$K+\frac{1}{2}$	$\frac{3}{2(l+1)(4l^2-1)}$	$\frac{3}{280}$	$\frac{1}{210}$	$\frac{3l}{2(l+1)(2l+1)}$	$\frac{9}{56}$
		l	$K-\frac{1}{2}$	$\frac{3(l+1)}{2l(2l+1)}$	$\frac{2}{7}$	$\frac{5}{24}$	$\frac{3}{2l(2l+1)(2l+3)}$	$\frac{1}{126}$
		$l-1$	$K+\frac{1}{2}$	$\frac{3(6l^3-l^2-1)}{2l(2l-1)^2(2l+1)}$	$\frac{76}{175}$	$\frac{367}{1176}$	$\frac{3(l+1)(2l-1)}{2l(2l+1)(2l+3)}$	$\frac{10}{63}$
		$l-1$	$K-\frac{1}{2}$	$\frac{3(l-1)}{2(2l-1)^2}$	$\frac{3}{25}$	$\frac{9}{98}$	0	0
	2	$l+2$	$K+\frac{1}{2}$	0	0	0	0	0
		$l+2$	$K-\frac{1}{2}$	0	0	0	$\frac{3(2l+5)}{(2l+3)^2}$	$\frac{11}{27}$
		$l+1$	$K+\frac{1}{2}$	0	0	0	$\frac{3l}{2(2l+3)^2}$	$\frac{1}{18}$
		$l+1$	$K-\frac{1}{2}$	$\frac{3(l+2)(2l+3)}{2(l+1)(4l^2-1)}$	$\frac{27}{56}$	$\frac{11}{35}$	$\frac{3l(l+2)(6l+11)}{2(l+1)(2l+1)(2l+3)^2}$	$\frac{145}{504}$
		l	$K+\frac{1}{2}$	$\frac{(2l+3)}{2(l+1)(2l+1)}$	$\frac{9}{56}$	$\frac{11}{90}$	$\frac{l(2l-1)(6l+11)}{2(l+1)(2l+1)(2l+3)^2}$	$\frac{145}{1512}$
		l	$K-\frac{1}{2}$	$\frac{(2l+3)(l+1)(6l-5)}{2(2l-1)^2(2l+1)l}$	$\frac{78}{175}$	$\frac{1045}{3528}$	$\frac{2l-1}{2l(2l+1)}$	$\frac{5}{42}$
		$l-1$	$K+\frac{1}{2}$	$\frac{3(l^2-1)(6l-5)}{2l(2l-1)^2(2l+1)}$	$\frac{52}{175}$	$\frac{95}{392}$	$\frac{3(l-1)(2l-1)}{2l(2l+1)(2l+3)}$	$\frac{5}{63}$
		$l-1$	$K-\frac{1}{2}$	$\frac{3(l+1)}{2(2l-1)^2}$	$\frac{6}{25}$	$\frac{15}{98}$	0	0

2 c *(cont.)*

J_{12}	K	J	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
2	$l-2$	$K+\frac{1}{2}$	$\frac{3(2l-3)}{(2l-1)^2}$	$\frac{9}{25}$	$\frac{15}{49}$	0	0	0
	$l-2$	$K-\frac{1}{2}$	0	0	0	0	0	0
2	$l+2$	$K\pm\frac{1}{2}$	0	0	0	$\frac{6(l+1)}{(2l+3)^2}$	$\frac{8}{27}$	$\frac{30}{121}$
	$l+1$	$K\pm\frac{1}{2}$	0	0	0	$\frac{3l}{(2l+3)^2}$	$\frac{1}{9}$	$\frac{12}{121}$
	l	$K\pm\frac{1}{2}$	$\frac{(l+1)(2l+3)}{(2l-1)^2(2l+1)}$	$\frac{36}{175}$	$\frac{55}{441}$	$\frac{l(2l-1)}{(2l+3)^2(2l+1)}$	$\frac{5}{189}$	$\frac{28}{1089}$
	$l-1$	$K\pm\frac{1}{2}$	$\frac{3(l+1)}{(2l-1)^2}$	$\frac{12}{25}$	$\frac{15}{49}$	0	0	0
	$l-2$	$K\pm\frac{1}{2}$	$\frac{6l}{(2l-1)^2}$	$\frac{18}{25}$	$\frac{24}{49}$	0	0	0

Table 1 contains as special cases the results Yamanouchi has obtained in [1] for p^4p and p^4d configurations. We get the corresponding values if we put $l=1$ and $l=2$ in table 1. At the first sight, his results seem to be quite different from ours. However, if we multiply our expressions with a suitable factor and (for the $\bar{g}_\lambda$:s) add another number, we arrive at exactly the same results as Yamanouchi except for some signs in the non-diagonal terms which, however, do not affect the energy values they give. (E.g. for $l=1$ multiplying the $\bar{g}_2$:s in table 1 a with 50 and adding -10 we get the same values as are given in [1] for the corresponding terms of the p^4p configuration.) This difference in the result can be traced back to a different definition of the integrals F^λ and G^λ. Further, the additive constant in $\bar{g}_\lambda$ depends on our having dropped a zero-point energy term in Eq. (43). In this way, we see that there is complete agreement between Yamanouchi's results and ours.

Pair coupling

Until now, we have only considered LS coupling. Now we are going to investigate how our results are modified if we assume a spin-orbit interaction giving rise to the coupling scheme (see [2]): $|(s_1\, s_2)\, S_{12},\, (l_1\, l_2)\, L_{12},\, J_{12},\, l_3,\, K,\, s_3,\, J\rangle$. The relation between this coupling scheme and LS coupling can be found by repeated use of (14):

2 d. Non-diagonal $\bar{g}'_\lambda$. $J = l - \frac{1}{2}$.

Parents		J_{12}	K	J'_{12}	K'	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
^1S	^3P	0	l	0	l	$\frac{\sqrt{2}\,(l+1)}{4l^2-1}$	$\frac{4\sqrt{2}}{35}$	$\frac{5\sqrt{2}}{63}$	$-\frac{\sqrt{2}\,(l+1)}{(2l+1)(2l+3)}$	$-\frac{4\sqrt{2}}{63}$	$-\frac{5\sqrt{2}}{99}$
				1	l	$-\frac{\sqrt{3}\sqrt{l+1}}{\sqrt{l}\,(4l^2-1)}$	$-\frac{2}{35}$	$-\frac{\sqrt{15}}{126}$	$\frac{\sqrt{3}\sqrt{l+1}}{\sqrt{l}\,(2l+1)(2l+3)}$	$\frac{2}{63}$	$\frac{\sqrt{15}}{198}$
				1	$l-1$	$-\frac{\sqrt{3}\,(l+1)}{\sqrt{l(2l-1)}\,(2l+1)}$	$-\frac{4\sqrt{5}}{35}$	$-\frac{5\sqrt{21}}{126}$	$\frac{\sqrt{3}\sqrt{2l-1}\,(l+1)}{\sqrt{l}\,(2l+1)(2l+3)}$	$\frac{4\sqrt{5}}{63}$	$\frac{5\sqrt{21}}{198}$
				2	l	$-\frac{\sqrt{(l+1)(2l+3)}}{\sqrt{l(2l-1)}\,(2l+1)}$	$-\frac{2\sqrt{15}}{35}$	$-\frac{\sqrt{385}}{126}$	$\frac{\sqrt{(l+1)(2l-1)}}{\sqrt{l(2l+3)}\,(2l+1)}$	$\frac{2\sqrt{15}}{63}$	$\frac{\sqrt{385}}{198}$
				2	$l-1$	$-\frac{\sqrt{3}\sqrt{(l-1)(l+1)}}{\sqrt{l(2l-1)}\,(2l+1)}$	$-\frac{2\sqrt{10}}{35}$	$-\frac{\sqrt{35}}{42}$	$\frac{\sqrt{3}\sqrt{(l-1)(l+1)(2l-1)}}{\sqrt{l}\,(2l+1)(2l+3)}$	$\frac{2\sqrt{10}}{63}$	$\frac{\sqrt{35}}{66}$
^1S	^1D	0	l	2	l	$\frac{\sqrt{2}\sqrt{l(l+1)(2l+3)}}{(2l+1)(2l-1)^{3/2}}$	$\frac{6\sqrt{30}}{175}$	$\frac{2\sqrt{770}}{441}$	$\frac{\sqrt{2}\sqrt{l(l+1)(2l-1)}}{(2l+1)(2l+3)^{3/2}}$	$\frac{2\sqrt{30}}{189}$	$\frac{2\sqrt{770}}{1089}$
^3P	^1D	0	l	2	l	$\frac{\sqrt{2l+3}\,(l+1)^{3/2}}{\sqrt{l}\,(2l+1)(2l-1)^{3/2}}$	$\frac{8\sqrt{15}}{175}$	$\frac{5\sqrt{385}}{882}$	$-\frac{\sqrt{l(l+1)(2l-1)}}{(2l+1)(2l+3)^{3/2}}$	$-\frac{2\sqrt{15}}{189}$	$-\frac{2\sqrt{385}}{1089}$
		0	l	2	$l-1$	$\frac{\sqrt{3}\sqrt{(l-1)(l+1)}}{\sqrt{l}\,(2l-1)^{3/2}}$	$\frac{2\sqrt{10}}{25}$	$\frac{3\sqrt{35}}{98}$	0	0	0
		1	l	2	l	$-\frac{\sqrt{3}\sqrt{2l+3}\,(l+1)}{\sqrt{2}\,l\,(2l+1)(2l-1)^{3/2}}$	$-\frac{2\sqrt{30}}{175}$	$-\frac{5\sqrt{462}}{3528}$	$\frac{\sqrt{3}\sqrt{2l-1}}{\sqrt{2}\,(2l+1)(2l+3)^{3/2}}$	$\frac{\sqrt{30}}{378}$	$\frac{\sqrt{462}}{2178}$
						$3\sqrt{l-1}\,(l+1)$	$4\sqrt{5}$	$15\sqrt{42}$			

						$\sqrt{2}\,l\,(4l^2-1)$	35	504	$\sqrt{2}\,(2l+1)\,(2l+3)^{3/2}$	189	2178
		1	$l-1$	2	$l-1$	$-\frac{3\sqrt{l+1}\,(l-1)^{3/2}}{\sqrt{2}\,l\,(2l-1)^2}$	$-\frac{4}{25}$	$-\frac{9\sqrt{30}}{392}$	0	0	0
		2	l	2	l	$-\frac{(l+1)\,(2l+3)}{\sqrt{2}\,(4l^2-1)\,l}$	$-\frac{6\sqrt{2}}{35}$	$-\frac{55\sqrt{2}}{504}$	$\frac{2l-1}{\sqrt{2}\,(2l+1)\,(2l+3)}$	$\frac{5\sqrt{2}}{126}$	$\frac{7\sqrt{2}}{198}$
		2	l	2	$l-1$	$\frac{\sqrt{3}\sqrt{(l-1)\,(2l+3)\,(l+1)}}{\sqrt{2}\,l\,(2l-1)^2}$	$\frac{4\sqrt{3}}{25}$	$\frac{15\sqrt{22}}{392}$	0	0	0
		2	$l-1$	2	l	$-\frac{\sqrt{3}\sqrt{(l-1)\,(2l+3)\,(l+1)}}{\sqrt{2}\,l\,(4l^2-1)}$	$-\frac{4\sqrt{3}}{35}$	$-\frac{5\sqrt{22}}{168}$	$\frac{\sqrt{3}\sqrt{l-1}\,(2l-1)}{\sqrt{2}\,(2l+1)\,(2l+3)^{3/2}}$	$\frac{5\sqrt{3}}{189}$	$\frac{7\sqrt{22}}{726}$
		2	$l-1$	2	$l-1$	$\frac{3\,(l-1)\,(l+1)}{\sqrt{2}\,l\,(2l-1)^3}$	$\frac{4\sqrt{2}}{25}$	$\frac{45\sqrt{2}}{392}$	0	0	0
^3P	^3P	0	l	1	l	$-\frac{\sqrt{6}\sqrt{l\,(l+1)}}{4l^2-1}$	$-\frac{6\sqrt{2}}{35}$	$-\frac{2\sqrt{30}}{63}$	$-\frac{\sqrt{3}\sqrt{l+1}}{\sqrt{2}\sqrt{l}\,(2l+1)\,(2l+3)}$	$-\frac{\sqrt{2}}{63}$	$-\frac{\sqrt{30}}{396}$
		0	l	1	$l-1$	$-\frac{2\sqrt{6}\,l^{3/2}}{(2l+1)\,(2l-1)^{3/2}}$	$-\frac{18\sqrt{10}}{175}$	$-\frac{16\sqrt{42}}{441}$	$-\frac{\sqrt{3}\sqrt{2l-1}\,(l+1)}{\sqrt{2}\sqrt{l}\,(2l+1)\,(2l+3)}$	$-\frac{2\sqrt{10}}{63}$	$-\frac{5\sqrt{42}}{396}$
		0	l	2	l	$-\frac{\sqrt{2}\sqrt{(l+1)\,(2l+3)}}{\sqrt{l}\,(2l+1)\,(2l-1)^{3/2}}$	$-\frac{2\sqrt{30}}{175}$	$-\frac{\sqrt{770}}{882}$	$-\frac{\sqrt{(l+1)\,(2l-1)}}{\sqrt{2}\sqrt{l}\,(2l+3)\,(2l+1)}$	$-\frac{\sqrt{30}}{63}$	$-\frac{\sqrt{770}}{396}$
		0	l	2	$l-1$	$-\frac{\sqrt{6}\sqrt{(l-1)\,(l+1)}}{\sqrt{l}\,(2l+1)\,(2l-1)^{3/2}}$	$-\frac{4\sqrt{5}}{175}$	$-\frac{\sqrt{70}}{294}$	$-\frac{\sqrt{3}\sqrt{(l-1)\,(l+1)\,(2l-1)}}{\sqrt{2}\sqrt{l}\,(2l+1)\,(2l+3)}$	$-\frac{2\sqrt{5}}{63}$	$-\frac{\sqrt{70}}{132}$
		1	l	1	$l-1$	$\frac{3\sqrt{l+1}\,(2l^2-l+1)}{2l\,(2l+1)\,(2l-1)^{3/2}}$	$\frac{16\sqrt{5}}{175}$	$\frac{87\sqrt{35}}{3528}$	$\frac{3\sqrt{(l+1)\,(2l-1)}}{2l\,(2l+1)\,(2l+3)}$	$\frac{\sqrt{5}}{63}$	$\frac{\sqrt{35}}{264}$
		1	l	2	l	$-\frac{\sqrt{3}\sqrt{2l+3}\,(l+1)\,(2l-3)}{2l\,(2l+1)\,(2l-1)^{3/2}}$	$-\frac{6\sqrt{15}}{175}$	$-\frac{25\sqrt{231}}{3528}$	$\frac{\sqrt{3}\sqrt{2l-1}}{2\sqrt{2l+3}\,l\,(2l+1)}$	$\frac{\sqrt{15}}{126}$	$\frac{\sqrt{231}}{792}$

Table 2 d *(cont.)*

Parents		J_{12}	K	J'_{12}	K'	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
		1	l	2	$l-1$	$-\frac{3\sqrt{l-1}\,(l+1)(2l-3)}{2l(2l+1)(2l-1)^{3/2}}$	$-\frac{6\sqrt{10}}{175}$	$-\frac{25\sqrt{21}}{1176}$	$\frac{3\sqrt{(l-1)(2l-1)}}{2l(2l+1)(2l+3)}$	$\frac{\sqrt{10}}{126}$	$\frac{\sqrt{21}}{264}$
		1	$l-1$	2	l	$\frac{\sqrt{3}\sqrt{(l+1)(2l+3)(2l^2+3l-3)}}{2l(2l+1)(2l-1)^2}$	$\frac{24\sqrt{3}}{175}$	$\frac{41\sqrt{165}}{3528}$	$\frac{\sqrt{3}\sqrt{l+1}\,(2l-1)}{2\sqrt{2l+3}\,l(2l+1)}$	$\frac{5\sqrt{3}}{63}$	$\frac{7\sqrt{165}}{792}$
		1	$l-1$	2	$l-1$	$\frac{3\sqrt{(l-1)(l+1)(2l^2+3l-3)}}{2l(2l+1)(2l-1)^2}$	$\frac{24\sqrt{2}}{175}$	$\frac{41\sqrt{15}}{1176}$	$\frac{3\sqrt{(l-1)(l+1)(2l-1)}}{2l(2l+1)(2l+3)}$	$\frac{5\sqrt{2}}{63}$	$\frac{7\sqrt{15}}{264}$
		2	l	2	$l-1$	$\frac{\sqrt{3}\sqrt{(l-1)(2l+3)(l+1)(6l-5)}}{2l(2l+1)(2l-1)^2}$	$\frac{26\sqrt{6}}{175}$	$\frac{95\sqrt{11}}{1176}$	$\frac{\sqrt{3}\sqrt{l-1}\,(2l-1)}{2\sqrt{2l+3}\,l(2l+1)}$	$\frac{5\sqrt{6}}{126}$	$\frac{7\sqrt{11}}{264}$

2 d. Non-diagonal $\bar{g}'_{\lambda}$. $J=l-\frac{3}{2}$.

Parents		J_{12}	K	J'_{12}	K'	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
^3P	^1D	1	$l-1$	2	$l-1$	$\frac{3\sqrt{(l-1)(l+1)}}{\sqrt{2}(2l-1)^2}$	$\frac{6}{25}$	$\frac{3\sqrt{30}}{98}$	0	0	0
^3P	^1D	2	$l-1$	2	$l-1$	$-\frac{3(l+1)}{\sqrt{2}(2l-1)^2}$	$-\frac{6\sqrt{2}}{25}$	$-\frac{15\sqrt{2}}{98}$	0	0	0
^3P	^1D	2	$l-2$	2	$l-1$	$-\frac{3\sqrt{(l+1)(2l-3)}}{(2l-1)^2}$	$-\frac{6\sqrt{3}}{25}$	$-\frac{15}{49}$	0	0	0
^3P	^3P	1	$l-1$	2	$l-1$	$-\frac{3\sqrt{(l-1)(l+1)}}{2(2l-1)^2}$	$-\frac{3\sqrt{2}}{25}$	$-\frac{3\sqrt{15}}{98}$	0	0	0
^3P	^3P	1	$l-1$	2	$l-2$	$-\frac{3\sqrt{(l-1)(2l-3)}}{\sqrt{2}(2l-1)^2}$	$-\frac{3\sqrt{3}}{25}$	$-\frac{3\sqrt{30}}{98}$	0	0	0
^3P	^3P	2	$l-1$	2	$l-2$	$3\sqrt{(l+1)(2l-3)}$	$3\sqrt{6}$	$15\sqrt{2}$	0	0	0

2

Parents		J_{12}	K	J'_{12}	K'	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
^1S	^3P	0	l	0	l	$-\frac{\sqrt{2}\,l}{4l^2-1}$	$-\frac{3\sqrt{2}}{35}$	$-\frac{4\sqrt{2}}{63}$	$\frac{\sqrt{2}\,l}{(2l+1)(2l+3)}$	$\frac{\sqrt{2}}{21}$	$\frac{4\sqrt{2}}{99}$
				1	$l+1$	$-\frac{\sqrt{3}\,l\sqrt{2l+3}}{\sqrt{l+1}\,(4l^2-1)}$	$-\frac{9\sqrt{3}}{70}$	$-\frac{4\sqrt{165}}{315}$	$\frac{\sqrt{3}\,l}{\sqrt{(l+1)(2l+3)(2l+1)}}$	$\frac{\sqrt{3}}{14}$	$\frac{4\sqrt{165}}{495}$
				1	l	$\frac{\sqrt{3}\sqrt{l}}{\sqrt{l+1}\,(4l^2-1)}$	$\frac{3}{70}$	$\frac{2\sqrt{15}}{315}$	$-\frac{\sqrt{3}\sqrt{l}}{\sqrt{l+1}\,(2l+1)(2l+3)}$	$-\frac{1}{42}$	$-\frac{2\sqrt{15}}{495}$
				2	$l+1$	$\frac{\sqrt{3}\sqrt{l(l+2)(2l+3)}}{\sqrt{l+1}\,(4l^2-1)}$	$\frac{9\sqrt{5}}{70}$	$\frac{2\sqrt{110}}{105}$	$-\frac{\sqrt{3}\sqrt{l(l+2)}}{\sqrt{(l+1)(2l+3)(2l+1)}}$	$-\frac{\sqrt{5}}{14}$	$-\frac{2\sqrt{110}}{165}$
				2	l	$\frac{\sqrt{l(2l+3)}}{\sqrt{(l+1)(2l-1)(2l+1)}}$	$\frac{3\sqrt{15}}{70}$	$\frac{2\sqrt{385}}{315}$	$-\frac{\sqrt{l(2l-1)}}{\sqrt{(l+1)(2l+3)(2l+1)}}$	$-\frac{\sqrt{15}}{42}$	$-\frac{2\sqrt{385}}{495}$
^1S	^1D	0	l	2	l	$\frac{\sqrt{2}\sqrt{l(l+1)(2l+3)}}{(2l-1)^{3/2}(2l+1)}$	$\frac{6\sqrt{30}}{175}$	$\frac{2\sqrt{770}}{441}$	$\frac{\sqrt{2}\sqrt{l(2l-1)(l+1)}}{(2l+3)^{3/2}(2l+1)}$	$\frac{2\sqrt{30}}{189}$	$\frac{2\sqrt{770}}{1089}$
^3P	^1D	0	l	2	$l+1$	0	0	0	$\frac{\sqrt{3}\sqrt{l(l+2)}}{\sqrt{l+1}\,(2l+3)^{3/2}}$	$\frac{\sqrt{5}}{18}$	$\frac{6\sqrt{110}}{605}$
		0	l	2	l	$-\frac{\sqrt{l(l+1)(2l+3)}}{(2l+1)(2l-1)^{3/2}}$	$-\frac{6\sqrt{15}}{175}$	$-\frac{2\sqrt{385}}{441}$	$\frac{\sqrt{2l-1}\,l^{3/2}}{\sqrt{l+1}\,(2l+1)(2l+3)^{3/2}}$	$\frac{\sqrt{15}}{126}$	$\frac{8\sqrt{385}}{5445}$
		1	$l+1$	2	$l+1$	0	0	0	$\frac{3\sqrt{l}\,(l+2)^{3/2}}{\sqrt{2}\,(l+1)(2l+3)^2}$	$\frac{5\sqrt{30}}{216}$	$\frac{36\sqrt{3}}{605}$
		1	$l+1$	2	l	$-\frac{\sqrt{3}\sqrt{l}\,(2l+3)}{\sqrt{2}\,(2l+1)(2l-1)^{3/2}}$	$-\frac{27\sqrt{10}}{350}$	$-\frac{11\sqrt{42}}{441}$	$\frac{\sqrt{3}\sqrt{2l-1}\,l^{3/2}}{\sqrt{2}\,(l+1)(2l+1)(2l+3)}$	$\frac{\sqrt{10}}{56}$	$\frac{4\sqrt{42}}{495}$

Table 2 d *(cont.)*

Parents		J_{12}	K	J'_{12}	K'	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
		1	l	2	$l+1$	0	0	0	$\frac{3l\sqrt{l+2}}{\sqrt{2}(l+1)(2l+3)^{3/2}}$	$\frac{\sqrt{10}}{24}$	$\frac{12\sqrt{33}}{605}$
		1	l	2	l	$\frac{\sqrt{3}\sqrt{2l+3}}{\sqrt{2}(2l+1)(2l-1)^{3/2}}$	$\frac{3\sqrt{30}}{350}$	$\frac{\sqrt{462}}{882}$	$-\frac{\sqrt{3}\sqrt{2l-1}\,l}{\sqrt{2}(l+1)(2l+1)(2l+3)^{3/2}}$	$-\frac{\sqrt{30}}{504}$	$-\frac{2\sqrt{462}}{5445}$
		2	$l+1$	2	$l+1$	0	0	0	$\frac{3l(l+2)}{\sqrt{2}(l+1)(2l+3)^2}$	$\frac{5\sqrt{2}}{72}$	$\frac{36\sqrt{2}}{605}$
		2	$l+1$	2	l	$\frac{\sqrt{3}\sqrt{l+2}(2l+3)}{\sqrt{2}(2l+1)(2l-1)^{3/2}}$	$\frac{9\sqrt{6}}{70}$	$\frac{11\sqrt{7}}{147}$	$-\frac{\sqrt{3}\sqrt{(l+2)(2l-1)}\,l}{\sqrt{2}(l+1)(2l+1)(2l+3)}$	$-\frac{5\sqrt{6}}{168}$	$-\frac{4\sqrt{7}}{165}$
		2	l	2	$l+1$	0	0	0	$\frac{\sqrt{3}\sqrt{(l+2)(2l-1)}\,l}{\sqrt{2}(l+1)(2l+3)^2}$	$\frac{5\sqrt{6}}{216}$	$\frac{12\sqrt{7}}{605}$
		2	l	2	l	$\frac{(2l+3)}{\sqrt{2}(4l^2-1)}$	$\frac{9\sqrt{2}}{70}$	$\frac{11\sqrt{2}}{126}$	$-\frac{l(2l-1)}{\sqrt{2}(l+1)(2l+1)(2l+3)}$	$-\frac{5\sqrt{2}}{168}$	$-\frac{14\sqrt{2}}{495}$
^3P	^3P	0	l	1	$l+1$	$\frac{\sqrt{3}\sqrt{2l+3}\,l}{\sqrt{2}\sqrt{l+1}(4l^2-1)}$	$\frac{9\sqrt{6}}{140}$	$\frac{2\sqrt{330}}{315}$	$\frac{2\sqrt{6}(l+1)^{3/2}}{(2l+1)(2l+3)^{3/2}}$	$\frac{16\sqrt{6}}{189}$	$\frac{10\sqrt{330}}{1089}$
		0	l	1	l	$-\frac{\sqrt{3}\sqrt{l}}{\sqrt{2}\sqrt{l+1}(4l^2-1)}$	$-\frac{3\sqrt{2}}{140}$	$-\frac{\sqrt{30}}{315}$	$\frac{\sqrt{6}\sqrt{l(l+1)}}{(2l+1)(2l+3)}$	$\frac{2\sqrt{2}}{21}$	$\frac{2\sqrt{30}}{99}$
		0	l	2	$l+1$	$-\frac{\sqrt{3}\sqrt{l(l+2)(2l+3)}}{\sqrt{2}\sqrt{l+1}(4l^2-1)}$	$-\frac{9\sqrt{10}}{140}$	$-\frac{2\sqrt{55}}{105}$	$\frac{\sqrt{6}\sqrt{l(l+2)}}{\sqrt{l+1}(2l+1)(2l+3)^{3/2}}$	$\frac{\sqrt{10}}{126}$	$\frac{4\sqrt{55}}{1815}$
		0	l	2	l	$-\frac{\sqrt{l(2l+3)}}{\sqrt{2}\sqrt{(l+1)(2l-1)}(2l+1)}$	$-\frac{3\sqrt{30}}{140}$	$-\frac{\sqrt{770}}{315}$	$\frac{\sqrt{2}\sqrt{l(2l-1)}}{\sqrt{l+1}(2l+1)(2l+3)^{3/2}}$	$\frac{\sqrt{30}}{378}$	$\frac{2\sqrt{770}}{5445}$
						$3\sqrt{l(2l+3)}$	$9\sqrt{3}$	$\sqrt{11}$	$3\sqrt{l}(2l^2+5l+4)$	$37\sqrt{3}$	$56\sqrt{11}$

					$\frac{}{2(l+1)(2l-1)(2l+1)}$	$\frac{}{280}$	$-\frac{}{105}$	$-\frac{}{2(l+1)(2l+1)(2l+3)^2}$	$-\frac{}{1512}$	$-\frac{}{1815}$
		1	$l+1$	2	l	$-\frac{\sqrt{3}\sqrt{l}\,(2l+3)}{2\sqrt{2l-1}\,(l+1)(2l+1)}$	$-\frac{27\sqrt{5}}{280}$	$-\frac{11\sqrt{21}}{315}$	$-\frac{\sqrt{3}\sqrt{l(2l-1)}\,(2l^2+l-4)}{2(l+1)(2l+1)(2l+3)^2}$	$-\frac{17\sqrt{5}}{1512}$	$-\frac{32\sqrt{21}}{5445}$
		1	l	2	$l+1$	$\frac{3\sqrt{(l+2)(2l+3)}}{2(l+1)(4l^2-1)}$	$\frac{9\sqrt{5}}{280}$	$\frac{\sqrt{66}}{210}$	$\frac{3\sqrt{l+2}\,l(2l+5)}{2(l+1)(2l+1)(2l+3)^{3/2}}$	$\frac{11\sqrt{5}}{168}$	$\frac{26\sqrt{66}}{1815}$
		1	l	2	l	$\frac{\sqrt{3}\sqrt{2l+3}}{2\sqrt{2l-1}\,(l+1)(2l+1)}$	$\frac{3\sqrt{15}}{280}$	$\frac{\sqrt{231}}{630}$	$\frac{\sqrt{3}\sqrt{2l-1}\,l(2l+5)}{2(l+1)(2l+1)(2l+3)^{3/2}}$	$\frac{11\sqrt{15}}{504}$	$\frac{26\sqrt{231}}{5445}$
		2	$l+1$	2	l	$\frac{\sqrt{3}\sqrt{l+2}\,(2l+3)}{2\sqrt{2l-1}\,(l+1)(2l+1)}$	$\frac{9\sqrt{3}}{56}$	$\frac{11\sqrt{14}}{210}$	$\frac{\sqrt{3}\sqrt{(l+2)(2l-1)}\,(6l+11)\,l}{2(l+1)(2l+1)(2l+3)^2}$	$\frac{145\sqrt{3}}{1512}$	$\frac{14\sqrt{14}}{363}$

2 d. Non-diagonal $\bar{g}'_{\lambda}$. $J = l + \frac{3}{2}$.

Parents		J_{12}	K	J'_{12}	K'	$4\bar{g}'_{l-1}$	$l=3$	$l=4$	$4\bar{g}'_{l+1}$	$l=3$	$l=4$
^3P	^1D	1	$l+1$	2	$l+1$	0	0	0	$-\frac{3\sqrt{l(l+2)}}{\sqrt{2}\,(2l+3)^2}$	$-\frac{\sqrt{30}}{54}$	$-\frac{6\sqrt{3}}{121}$
^3P	^1D	2	$l+2$	2	$l+1$	0	0	0	$-\frac{3\sqrt{l(2l+5)}}{(2l+3)^2}$	$-\frac{\sqrt{33}}{27}$	$-\frac{6\sqrt{13}}{121}$
^3P	^1D	2	$l+1$	2	$l+1$	0	0	0	$-\frac{3l}{\sqrt{2}\,(2l+3)^2}$	$-\frac{\sqrt{2}}{18}$	$-\frac{6\sqrt{2}}{121}$
^3P	^3P	1	$l+1$	2	$l+2$	0	0	0	$\frac{3\sqrt{(l+2)(2l+5)}}{\sqrt{2}\,(2l+3)^2}$	$\frac{\sqrt{110}}{54}$	$\frac{3\sqrt{39}}{121}$
^3P	^3P	1	$l+1$	2	$l+1$	0	0	0	$\frac{3\sqrt{l(l+2)}}{2(2l+3)^2}$	$\frac{\sqrt{15}}{54}$	$\frac{3\sqrt{6}}{121}$
^3P	^3P	2	$l+2$	2	$l+1$	0	0	0	$\frac{3\sqrt{l(2l+5)}}{\sqrt{2}\,(2l+3)^2}$	$\frac{\sqrt{66}}{54}$	$\frac{3\sqrt{26}}{121}$

$$|(s_1\, s_2)\, S_{12},\ (l_1\, l_2)\, L_{12},\ J_{12},\ l_3,\ K,\ s_3,\ J\rangle = \sum_{L_{123}} (-1)^{S_{12}+L_{12}+l_3+K} \begin{Bmatrix} S_{12} & L_{12} & J_{12} \\ l_3 & K & L_{123} \end{Bmatrix} \cdot$$

$$\cdot\, [2\, J_{12}+1)\,(2\, L_{123}+1)]^{\frac{1}{2}}\, |(s_1\, s_2)\, S_{12},\ [(l_1\, l_2)\, L_{12},\ l_3]\, L_{123},\ K,\ s_3,\ J\rangle = (-1)^{l_3+L_{12}} \sum_{L_{123}} (-1)^{L_{123}} \cdot$$

$$\cdot \begin{Bmatrix} S_{12} & L_{12} & J_{12} \\ l_3 & K & L_{123} \end{Bmatrix} [(2\, J_{12}+1)\,(2\, L_{123}+1)]^{\frac{1}{2}}\, |[(l_1\, l_2)\, L_{12},\ l_3]\, L_{123},\ (s_1\, s_2)\, S_{12},\ K,\ s_3,\ J\rangle =$$

$$= (-1)^{l_3+L_{12}} \sum_{L_{123}} (-1)^{L_{123}} \begin{Bmatrix} S_{12} & L_{12} & J_{12} \\ l_3 & K & L_{123} \end{Bmatrix} [(2\, J_{12}+1)\,(2\, L_{123}+1)]^{\frac{1}{2}} \sum_{S_{123}} (-1)^{L_{123}+S_{12}+s_3+J} \cdot$$

$$\cdot \begin{Bmatrix} L_{123} & S_{12} & K \\ s_3 & J & S_{123} \end{Bmatrix} [(2\, K+1)\,(2\, S_{123}+1)]^{\frac{1}{2}}\, |[(l_1\, l_2)\, L_{12},\ l_3]\, L_{123},\ [(s_1\, s_2)\, S_{12},\ s_3]\, S_{123},\ J\rangle. \tag{56}$$

This formula allows us to use our earlier results for LS coupling in the following way

$$\langle (s_1\, s_2)\, S_{12},\ (l_1\, l_2)\, L_{12},\ J_{12},\ l_3,\ K,\ s_3,\ J \,|\sum_{k>l} \frac{e^2}{r_{kl}}|\, (s_1\, s_2)\, S'_{12},\ (l_1\, l_2)\, L'_{12},\ J'_{12},\ l_3,\ K',\ s_3,\ J\rangle =$$

$$= (-1)^{2l_3+L_{12}+L'_{12}} \sum_{\substack{L_{123}\\ L'_{123}}} \begin{Bmatrix} S_{12} & L_{12} & J_{12} \\ l_3 & K & L_{123} \end{Bmatrix} \begin{Bmatrix} S'_{12} & L'_{12} & J'_{12} \\ l_3 & K' & L'_{123} \end{Bmatrix} \cdot$$

$$\cdot\, [(2\, J_{12}+1)\,(2\, J'_{12}+1)\,(2\, L_{123}+1)\,(2\, L'_{123}+1)]^{\frac{1}{2}} (-1)^{S_{12}+S'_{12}+2(s_3+J)} \sum_{\substack{S_{123}\\ S'_{123}}} \begin{Bmatrix} L_{123} & S_{12} & K \\ s_3 & J & S_{123} \end{Bmatrix} \cdot$$

$$\cdot \begin{Bmatrix} L'_{123} & S'_{12} & K' \\ s_3 & J & S'_{123} \end{Bmatrix} [(2\, K+1)\,(2\, K'+1)\,(2\, S_{123}+1)\,(2\, S'_{123}+1)]^{\frac{1}{2}} \cdot$$

$$\cdot \langle (L_{12},\ l_3)\, L_{123},\ (S_{12},\ s_3)\, S_{123},\ J \,|\sum_{k>l} \frac{e^2}{r_{kl}}|\, (L'_{12},\ l_3)\, L'_{123},\ (S'_{12},\ s_3)\, S'_{123},\ J\rangle =$$

$$= 2\,\Big(\sum_{\lambda} - \bar{f}'_{\lambda}\, F^{\lambda} + \bar{g}'_{\lambda}\, G^{\lambda}\Big) + \text{energy of parent ion.} \tag{57}$$

The general expressions for $\bar{f}'_{\lambda}$ and $\bar{g}'_{\lambda}$ are given by .

$$\bar{f}'_{\lambda} = (-1)^{l+S_{12}+K+J_{12}+J'_{12}}\, (2\, l+1)\,(2\, l_v+1) \begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_v & l_v & \lambda \\ 0 & 0 & 0 \end{pmatrix} [(2\, J_{12}+1)\,(2\, J'_{12}+1) \cdot$$

$$\cdot\, (2\, L_{12}+1)\,(2\, L'_{12}+1)]^{\frac{1}{2}} \begin{Bmatrix} L_{12} & \lambda & L'_{12} \\ l & l & l \end{Bmatrix} \begin{Bmatrix} \lambda & L_{12} & L'_{12} \\ S_{12} & J'_{12} & J_{12} \end{Bmatrix} \begin{Bmatrix} J_{12} & \lambda & J'_{12} \\ l_v & K & l_v \end{Bmatrix} \delta_{S_{12}S'_{12}}\, \delta_{KK'} \tag{58}$$

and

$$\bar{g}'_{\lambda} = (-1)^{L_{12}+L'_{12}}\, (2\, l+1)\,(2\, l_v+1) \left[\begin{pmatrix} l & l_v & \lambda \\ 0 & 0 & 0 \end{pmatrix}\right]^2 [(2\, J_{12}+1)\,(2\, J'_{12}+1)\,(2\, K+1) \cdot$$

$$\cdot\, (2\, K'+1)\,(2\, L_{12}+1)\,(2\, L'_{12}+1)\,(2\, S_{12}+1)\,(2\, S'_{12}+1)]^{\frac{1}{2}} \sum_{\mathfrak{C}} (2\, \mathfrak{C}+1) \begin{Bmatrix} S_{12} & L_{12} & J_{12} \\ l_v & K & \mathfrak{C} \end{Bmatrix} \cdot$$

$$\cdot \begin{Bmatrix} S'_{12} & L'_{12} & J'_{12} \\ l_v & K' & \mathfrak{C} \end{Bmatrix} \begin{Bmatrix} \mathfrak{C} & S_{12} & K \\ \frac{1}{2} & J & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \mathfrak{C} & S'_{12} & K' \\ \frac{1}{2} & J & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} l & l & L_{12} \\ l_v & \mathfrak{C} & \lambda \end{Bmatrix} \begin{Bmatrix} l & l & L'_{12} \\ l_v & \mathfrak{C} & \lambda \end{Bmatrix}. \tag{59}$$

For our particular case of ArII with $l=1$ and l_v arbitrary the non-vanishing values of $\bar{f}'_\lambda$ and $\bar{g}'_\lambda$ are given in table 2.

In the practical applications of these results it must be remembered that the energy of the parent ion must always be added. The coefficients of the Coulomb- and exchange integrals for two holes in a p-shell is the same as for two p-electrons (see [3] p. 299) and are given e.g. in [3] p. 198. The spin-orbit energy for the same system can e.g. be found in table 1^{11} p. 268.

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REFERENCES

1. T. Yamanouchi, Proc. Phys.-Math. Soc. Japan *20*, 547 (1938); ibid., *21*, 47 (1939).
2. G. Racah, Phys. Rev. *61*, 537 (1942).
3. E. U. Condon and G. H. Shortley, "The Theory of Atomic Spectra". Cambridge 1935.
4. A. R. Edmonds, "Angular Momentum in Quantum Mechanics". Princeton 1957.
5. G. Racah, Phys. Rev. *61*, 186 (1942).
6. G. Racah, ibid., *62*, 438 (1942).
7. G. H. Shortley and B. Fried, Phys. Rev. *54*, 739 (1938).

Note added in proof. In Tables 2 c and 2 d, $4\,\bar{g}'_\lambda$ is tabulated instead of $2\,\bar{g}'_\lambda$. This is due to the fact that in proof-reading a factor of $\frac{1}{2}$ in the $\bar{g}'_\lambda$'s was found to have been omitted and it was too late to multiply the whole of the tables by $\frac{1}{2}$.

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